MULTIPHASE FLOW AND INTERACTION DYNAMICS
BETWEEN BENTONITE CLAY AND FRACTURED CRYSTALLINE ROCK

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ABSTRACT

Deep geological repositories are commonly considered as suitable environments for final disposal of high-level spent nuclear fuel. In the Swedish and Finnish repository design concept, copper canisters containing spent nuclear fuel are to be placed in deposition holes, as part of a system of deep underground tunnels in sparsely fractured crystalline bedrock, within which each canister is embedded with a bentonite-clay-mixture buffer in the deposition holes.

Bentonite is a porous, expansive clay material with low permeability that develops a relatively high swelling pressure when hydrated. The swelling acts to tightly embed and seal the canister in its deposition hole, minimizing void space and, combined with the low hydraulic conductivity of saturated bentonite, reducing advective water flow in the immediate vicinity of the canister. Also, the retention characteristics of bentonite limit particle dispersion, thereby acting as a formidable transport barrier. However, there are several unresolved issues related to the resaturation dynamics of bentonite in bedrock, in particular when in contact with water-conducting fractures in a strongly hetero-geneous and anisotropic sparsely fractured rock environment.

In this study, a set of semi-generic, radially symmetric TOUGH2 simulation experiments are conducted to investigate the resaturation and multiphase dynamics of water and air in a bentonite-rock environment, with a particular focus on the dynamics at the bentonite-rock interface. The main objective is to identify how sensitive resaturation times are to assumed constitutive relationships for relative permeabil-ity as a function of saturation, and to the geom-etry and properties of the rock fractures. A scenario analysis is carried out using the script-ing capabilities of the PYTOUGH library for optimum flexibility. This work will be further extended for use in combination with a suite of onsite subsurface tunnel experiments denoted as the Bentonite Rock Interaction Experiments (BRIE), currently being conducted at the Äspö Hard Rock Laboratory in Sweden. The main aims of the BRIE experiments are to identify and quantify interactions of water resaturation of bentonite clay under *in situ* conditions, that is, in a deep geological environment consisting of sparsely fractured rock similar to the candidate site for the final repository in Sweden.

Preliminary results identify fracture geometry as a primary factor affecting the resaturation time. The parameterization of the gas permeability appears as very important for correctly rendering the behavior close to saturation, the domain in which most uncertainties remain.

INTRODUCTION

Management and disposal of high-level spent nuclear fuel is an open question in countries that rely on nuclear power. An envisaged solution is to build final repositories in deep geological formations. The underlying idea is that such underground environments, where transport mechanisms are slow, would act as a natural barrier and delay the release of the decaying waste for a sufficient amount of time in the event of a failure of the engineered containers.

The Swedish repository design concept targets sparsely fractured granite bedrock as the host formation. In deep underground tunnels, vertical deposition holes would be drilled in the tunnel floor to receive copper canisters containing the nuclear waste. The deposition holes would be packed and the tunnels backfilled with a pre-

packed partially wetted bentonite clay mixture (Johannesson et al., 2007). Bentonite is a porous clay material with a complex microstructure depending heavily on its water content—a material that exhibits an overall swelling behavior when it rehydrates. The choice of an expansive clay material is made for several reasons: with its very low permeability and high-retention characteristics, bentonite would keep the advective transport to a minimum. Its high swelling pressure would seal void spaces in the back-fill material and contact points within the deposition hole and tunnel walls, as well as prevent the occurrence of bacterial activity as a possible corrosion enhancer in the canisters.

Despite its many advantageous features, predicting the behavior of a bentonite buffer embedded in fractured crystalline rock is a significant modeling challenge, due to the complex interactions between thermo-hydro-mechanical (THM) processes. The considered large-scale conditions point towards a full resaturation of the system in the long run, but we need to determine at what rate the originally unsaturated clay can take up water at the interface with the neighboring rock.

The fate of the air present in the originally unsaturated zone also has to be determined. Several possibilities could occur, like air entrapment in some regions of the buffer or in rock fractures, or a temporary desaturation of the rock mass in contact with the bentonite due to the very high affinity with water of the latter. The presence of intersecting rock fractures, their respective geometry and transmissivity, as well as the hydromechanical properties of the buffer are expected to play a major part in the above-mentioned features. The ongoing Bentonite Rock Interaction Experiment (BRIE) at the Äspö HRL in Sweden is conducted to achieve a better understanding of the dynamics and to gather modeling experience for such systems.

Several models are available at different levels of complexity. A common simplification is to use Richards' assumptions—that is, to neglect the air mass balance and treat the gas phase as a passive, perfectly mobile bystander. A more rigorous way is to use a two-component multi-phase flow model, which accounts for all thermo-hydrological (TH) processes for air and water present in gas and liquid form. Only the latter can help determine whether air entrapment is likely in the selected design, or what the possible extent and duration of system transient behavior might be. Further couplings can integrate the mechanical (M) aspects together with the hydrological dependence of the problem (Rutqvist et al., 2010).

This study investigates the influence of some of the abovementioned factors, namely the intersection of boreholes by fractures at different points, and the effect of different parameterizations of bentonite permeability to air. In this study, we use TOUGH2 with its two-component (air, water) equation-of-state module EOS3 to simulate bentonite resaturation in a simplified, semi-generic fractured rock setting, with an open tunnel and a deposition hole filled with bentonite. Specifically, we investigate the constitutive relationships for gas-phase relative permeability. The main model variables of interest in terms of results are the resaturation and gas pressure fields. These are analyzed in the bentonite and fractured rock regime close to the deposition hole. Results between the various assumed constitutive relationships for gas permeability are then compared.

METHOD

We choose to look primarily at hydrogeological (H) processes under isothermal conditions with help of the TOUGH2 multiphase flow code (Pruess et al., 1999). The underlying assumptions are that both water and air fluxes are described by Darcy's law generalized to multi-phase applications. Gases are described by the ideal gas law, and the total gas pressure is taken as the sum of the pressures of all the constituents (perfect mixing). Henry's law drives the dissolution/release of air into/from water. The capillary pressure and the relative permeability to gas and liquid are defined as characteristic curves. Closure relationships on water and air mass fractions and on liquid and gas saturations complete the system.

The water retention curves (capillary pressure as a function of liquid saturation) of the bentonite and the rock follow a van Genuchten curve as defined by the standard input in TOUGH2

(Pruess et al., 1999) using parameter values corresponding, respectively, to the properties of the commercial MX-80 bentonite mixture and to values reported as representative of the bedrock at the Äspö HRL in Sweden.

The mechanical (M) processes are not included directly but introduced instead as an alteration of the water retention curve of the bentonite (Dueck, 2004). A relationship linking the suction of the bentonite, here taken as the capillary pressure P_{cap}, i.e., the difference between the pressure in the gas and the liquid phase, under free swelling ($P_{cap\ free}$) and under confined conditions ($P_{cap\ conf}$), is proposed as follows (Dueck, 2004):

$$P_{cap\ conf}(w,P)= P_{cap\ free}(w) - \alpha \cdot P$$

where P is the mean stress, w is the water content and α has been reported numerically close to 1.0. Estimates of the capillary pressure under confined conditions are available through free capillary pressure data and free swelling data. The modification of the water retention properties of the bentonite due to swelling are integrated by calibrating the set of van Genuchten parameters against $P_{cap\ conf}$.

We undertook a scenario analysis to test the impact of the gas relative permeability on the bentonite (Table 1). The implemented alternative 1 comes from standard TOUGH2 input methods, and alternative 2 is fitted from field data reported in the literature (Alonso et al., 2005).

The first scenario respects the traditional concept of intrinsic permeability being allocated to the gas or liquid phase through varying relative permeability functions, with values ranging between 0 and 1. The second scenario, based on laboratory experiments, abandons this hypothesis and considers much higher permeability values for gas when liquid saturation is smaller than 90%. The corresponding permeability functions are presented in Figure 1. Scenarios 2, 3 and 4 collectively investigate what impact the point-of-intersection location has between the fracture and the deposition hole (Table 1). The last complementary scenarios, 5 and 6, add a new permeability definition (also present in Figure 1) and make use of Richards' equation by running EOS9. They will be key in the discussion below.

A radial geometry is configured according to Figure 2. The tunnel and the deposition hole are placed on the symmetry axis. A horizontal fracture intersects the deposition hole at mid-depth and is assigned effective hydraulic properties typical for Äspö granitic rock. Here, a constant effective hydraulic transmissivity of 5×10^{10} m^2/s is used. The mesh generation is performed with AMESH adopting an unconventional approach: the radial slice is taken as a layer with variable thickness.

Table 1. Description of the implanted scenarios

| Scenario	Description
1 (base)	Base scenario: EOS3, relative permeabilities in clay by standard Tough2 input reported from Fatt and Klikoff (1959) as reported in Pruess et al. (1999) (Fig. 1): $k_{rl}=S^3$: $k_{rg}=(1-S)^3$
2 (perm)	EOS3, permeabilities in clay to fit the lab-measured values reported in Alonso et al. (2005): $k_{rl}=S^3$: $k_{rg}=10^8.(1-S)^4$ (Fig. 1)
3 (permtop)	Similar to scenario 2 but fracture intersecting at the top of the deposition hole
4 (permbot)	Similar to scenario 2 but fracture intersecting at the bottom of the deposition hole
5 (perfmob) Qualitative results only	EOS3, permeabilities in clay by standard Tough2 input, with perfectly mobile gas and $k_{rl}=S^3$, $k_{rg}=1.0$ (Fig. 1)
6 (rich) Qualitative results only	EOS9, air is a passive bystander, permeability to liquid in clay by standard Tough2 input, $k_{rl}=S^3$
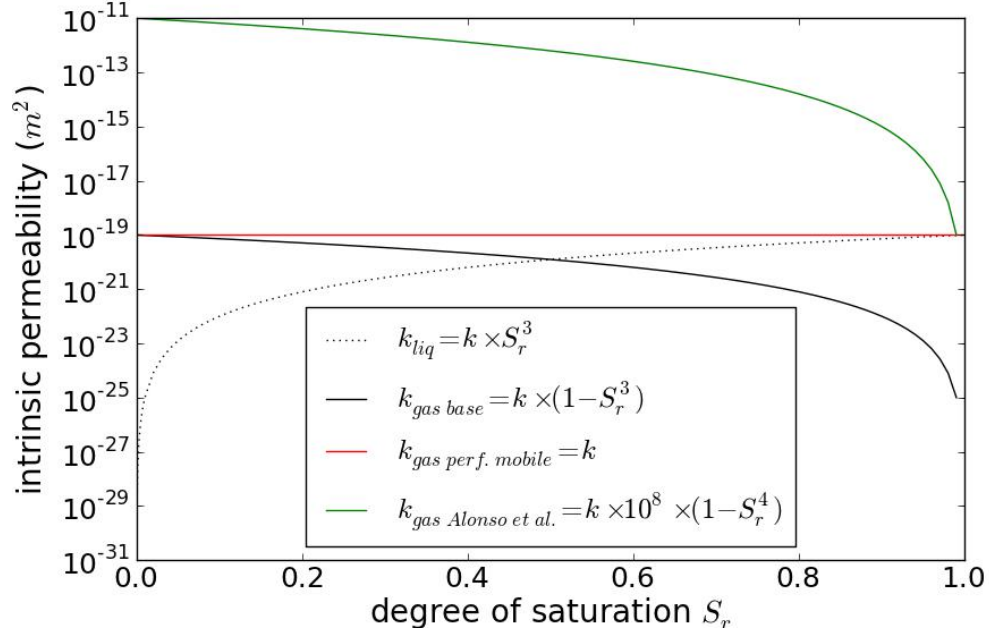
Figure 1. The constitutive relationships used for relative permeability of liquid (black dotted) and gas (solid) as a function of saturation. Scenario 5 adopts a constant relative permeability (red), scenarios 2, 3, and 4 adopt the approach used by Alonso et al. (2005) (green), and scenario 1 adopts a cubic power approach and is used as a reference base case for the simulations (black).
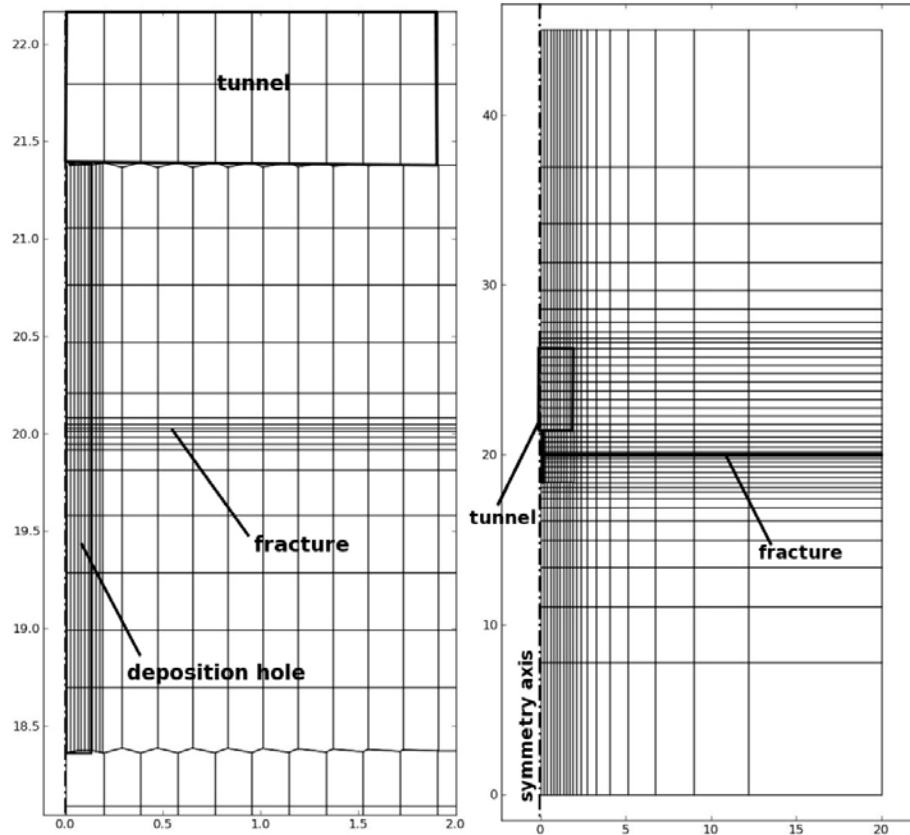

Figure 2. A radially symmetric domain is applied with a tunnel, deposition hole and fracture. The deposition hole consists of bentonite MX-80, the fracture consists of mesh elements with higher hydraulic conductivity K than the background rock matrix. The tunnel is implemented as a boundary condition with atmospheric pressure.

Interface areas are then corrected to approximate radial conditions, and the axes convention is switched back to its usual convention: vertical coordinate z and radial coordinate r.

The application uses the equation of state EOS3, which accounts for air and water present in gas and liquid phases. Fixed boundary conditions are imposed at the borders other than the symmetry axis and in the cells forming the tunnel: water saturation with pressure equal to 2.0 MPa for the outer boundaries and air saturation at atmospheric pressure is assumed in the tunnel.

For more flexibility in generating the different sets of TOUGH input files in the frame of this scenario analysis, the PYTHON programming language and the PYTOUGH library are used.

RESULTS AND ANALYSIS

The resaturation of the clay buffer is represented here by the time saturation S_r takes to reach a certain percentage in every cell in the lower half of the deposition hole. Results obtained for the bounds $S_r>50\%$, $S_r>90\%$ and $S_r>99\%$ are presented in Table 2. The simulation output frequency increases from one record per day initially to once every 10 days beyond $t=100$ days. We observe that the permeability definitions used in scenario 1 and 2 follow very close patterns up to 90% saturation.

The comparison of fracture locations via scenarios 2, 3, and 4 shows that the quickest resaturation event happens for case 2 (where the fracture intersects the middle of the deposition hole). This can be interpreted as the case when the longest flow path of water from the fracture outlet to any point in the deposition hole is minimal. This observation may indicate that the fracture considered has water-bearing properties on par with the background flow through the rock matrix to globally provide water to the system. This hypothesis could be verified by calculating the accumulated flow values through key vertical cross sections in the model.

Table 2. Time in days until all cells in the lower half of the deposition hole reach certain levels of water saturation

Scenario	$T_{50\%}$	$T_{90\%}$	$T_{99\%}$
1_base	140 d	180 d	>215 d
2_perm (middle)	140 d	180 d	>215 d
3_perm top	260 d	310 d	>330 d
4_perm bottom	240 d	320 d	>706 d

Comparing the differences between inflow from the top or the bottom, several influences come into play: the effect of gravity against capillarity forces, the proximity to the tunnel floor that might drain more water, and the possibility of air entrapment slowing down the full resaturation time. However, the similar outcome from both extremities could indicate that, in the current setup, the presence of a fracture within the studied range of transmissivity is not sensed further than 1.5 m away (half the height of the borehole) from the outlet during the first 300 days of the experiment. Water balance and analyses of the flow field should provide the opportunity to confirm or reject this idea.

The implementation of these scenarios also highlights some peculiar behavior related to the gas pressure in the clay buffer close to saturation. For simulation case 2, the gas pressure distribution after 215 days would indicate that the gas pressure in the deposition hole, then within the last few percent to full re-saturation, is ~3 MPa and hence actually exceeds the 2 MPa pressure imposed at the boundary (Fig. 3). Further investigations are required, since it has not yet been successfully linked to the swelling or to any other known effect related to pressure, such as the Klinkenberg effect or the vapor pressure lowering effect offered by EOS4. However, different assumptions such as a perfectly mobile gas (scenario 5) or simulations based on the Richards equation (scenario 6) did not demonstrate this particular feature. It is thus suspected that the ratio of permeability to
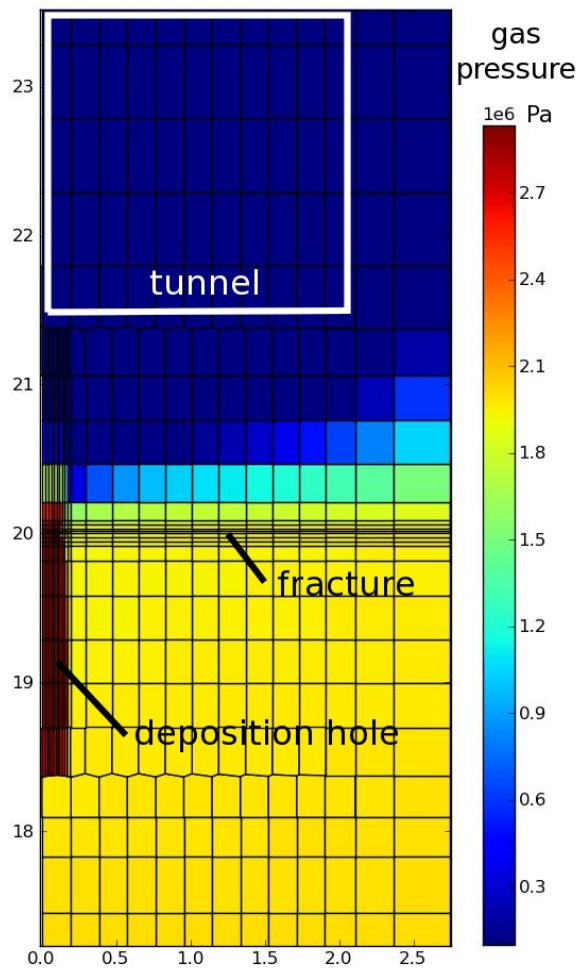
Figure 3. Gas pressure profile in the close field with scenario 2 after 215 days, the gas pressure in the bentonite domain exceeds the far field boundary value of 2 MPa.

gases over permeability to liquids is a key factor close to saturation. Hence, the area where unsaturated conditions approach full saturation is highly sensitive to the assumed constitutive relationship used, and as such, becomes all the more important for determining the risk of air entrapment.

SUMMARY AND CONCLUSIONS

In this initial study, resaturation effects and interactions between bentonite clay and sparsely fractured granitic rock is investigated. The main focus is to study the effects of constitutive relationships for gas permeability as a function of saturation. Three possible constitutive relationships have been investigated. We also analyzed the location of rehydration. The main results of this analysis show that:

- The location of the fractures around the deposition hole significantly influences the total time for resaturation. Interestingly, the central intersection location has the fastest rewetting time. This is attributed to combined gravitational and capillary re-wetting effects, since the flow-path distance to all points of the bentonite domain are minimized. Complementary investigations of fracture-network transmissivity and connectivity are required to deepen the understanding of that factor.

- The choice of permeability functions for gas in the bentonite seems to be determinant for behavior close to saturation. A better conceptual understanding of the processes and their parameterization in that regime is necessary. Modeling, together with the data generated by the BRIE experiments, will be an asset toward reaching this goal.

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